International Journal of
# Quantum Chemistry

## Contents for Volume 67, 1998

**Issue No. 1, 1998**

**Theoretical and Computational Developments**

A New Way of Analyzing Vibrational Spectra. I. Derivation of Adiabatic Internal Modes
*Z. Konkoli and D. Cremer* ..... **1**

A New Way of Analyzing Vibrational Spectra. II. Comparison of Internal Mode Frequencies
*Z. Konkoli, J. A. Larsson, and D. Cremer* ..... **11**

A New Way of Analyzing Vibrational Spectra. III. Characterization of Normal Vibrational Modes in Terms of Internal Vibrational Modes
*Z. Konkoli and D. Cremer* ..... **29**

A New Way of Analyzing Vibrational Spectra. IV. Application and Testingof Adiabatic Modes Within the Concept of the Characterization of Normal Modes
*Z. Konkoli, J. A. Larsson, and D. Cremer* ..... **41**

Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems of Spectral Resolution. IV
*S. Arimoto, K. Fukui, K. F. Taylor, and P. G. Mezey* ..... **57**

**Issue No. 2, 1998**

**Theoretical and Computational Developments**

New Bosonic Excitation Operators in Many-Electron Wave Functions
*K. Ohta* ..... **71**

On the Rapid Evaluation of Cofactors in the Calculation of Nonorthogonal Matrix Elements
*F. Dijkstra and J. H. Van Lenthe* ..... **77**

**Properties, Dynamics, and Electronic Structure of Atoms and Molecules**

On the Inverse Born–Oppenheimer Separation for High Rydberg States of Molecules
*F. Remacle and R. D. Levine* ..... **85**

Structure of the $T_1$-State Wave Function of Linear Polyenes
*O. Takahashi, M. Watanabe, and O. Kikuchi* ..... **101**

Role of $\pi$ Stabilization in Cyclic Polyenes
*S. Larsson and L. Rodríguez-Monge* ..... **107**

**Properties, Dynamics, and Electronic Structure of Condensed Systems and Clusters**

Coupled Cluster Treatments of Periodic Systems from Strongly Localized Reference Functions: 1-D and 2-D Spin and Electron Lattices
*B. Miguel, M. Cousy, and J.-P. Malrieu* ..... **115**

**Issue No. 3, 1998**

**Theoretical and Computational Developments**

Adiabatic Evolution of Eigenspectra of Model 1-D and 2-D Hamiltonians: Quantum Adiabatic Switching Algorithm in a Time-Independent Fourier Grid Hamiltonian Framework
*P. Sarkar and S. P. Bhattacharyya* ..... **133**

Correlation Potentials for the He Atom and the Hydrogen Molecule: A Comparison Between the Correlation Factor Approach and DFT Correlation Energy Functionals
*F. Moscardó and A. J. Pérez-Jiménez* ..... **143**

**Properties, Dynamics, and Electronic Structure of Atoms and Molecules**

Charge Fluctuations and Correlation Strength in Chemical Bonds: First-Row Homonuclear Diatomic Molecules
*M. Yu, M. Dolg, P. Fulde, and H. Stoll* ..... **157**

Cyanide Adsorbed on Coinage Metal Electrodes: A Relativistic Density Functional Investigation
*M.-S. Liao, X. Lü, and Q.-E. Zhang* ..... **175**

**Properties, Dynamics, and Electronic Structure of Condensed Systems and Clusters**

Theoretical Study of Fullerene Derivatives: $C_{28}H_4$ and $C_{28}X_4$ Cluster Molecules
*L.-H. Lu, K.-C. Sun, and C. Chen* ..... **187**

**Issue No. 4, 1998**

**Theoretical and Computational Developments**

Computation of Overlap Integrals Over Slater-Type Orbitals Using Auxiliary Functions
*I. I. Guseinov, A. Özmen, Ü. Atav, and H. Yüksel* ..... **199**

Model Study of the Impact of Orbital Choice on the Accuracy of Coupled-Cluster Energies. I. Single-Reference-State Formulation
*K. Jankowski, K. Kowalski, K. Rubiniec, and J. Wasilewski* ..... **205**

Model Study of the Impact of Orbital Choice on the Accuracy of Coupled-Cluster Energies. II. Valence-Universal Coupled-Cluster Method
*K. Jankowski, J. Gryniaków, and K. Rubiniec* ..... **221**

Model Study of the Impact of Orbital Choice on the Accuracy of Coupled-Cluster Energies. III. State-Universal Coupled-Cluster Method
*K. Jankowski, L. Meissner, and K. Rubiniec* ..... **239**

**Properties, Dynamics, and Electronic Structure of Atoms and Molecules**

Stripped Ion–Helium Atom Collision Dynamics Within a Time-Dependent Quantum Fluid Density Functional Theory
*B. K. Dey and B. M. Deb* ..... **251**

**Issue No. 5, 1998**

**Theoretical and Computational Developments**

Quantum Dynamics with Lanczos Subspace Propagation: Application to a Laser-Driven Molecular System
*C. S. Guiang and R. E. Wyatt* ..... **273**

Efficient Algorithm for the Spin-Free Valence Bond Theory. I. New Strategy and Primary Expressions
*W. Wu, A. Wu, Y. Mo, M. Lin, and Q. Zhang* ..... **287**

On the Use of Symmetry-Adapted Crystalline Orbitals in SCF-LCAO Periodic Calculations. I. The Construction of the Symmetrized Orbitals
*C. M. Zicovich-Wilson and R. Dovesi* ..... **299**

On the Use of Symmetry-Adapted Crystalline Orbitals in SCF-LCAO Periodic Calculations. II. Implementation of the Self-Consistent-Field Scheme and Examples
*C. M. Zicovich-Wilson and R. Dovesi* ..... **311**

Geometrically Active Atomic States and the Formation of Molecules in Their Normal Shapes
*C. A. Nicolaides and Y. Komninos* ..... **321**

**Molecular Structure, Dynamics, and Function of Biological Systems**

Ab Initio Assessment of the Electronic Structure of 5α-Reduced Progestins
*C. Kubli-Garfias* ..... **329**

**Book Review**

Dynamics of Molecules and Chemical Reactions. Edited by Robert E. Wyatt and John Z. Zhang
*E. Deumens* ..... **339**

**Erratum**

Conformational Analysis of Polypeptide Chains with the Aid of Density of States Calculations
*S. G. Jacchieri* ..... **341**

**Issue No. 6, 1998**

**Theoretical and Computational Developments**

Harmonic Oscillator Tensors. V. The Doubly Degenerate Harmonic Oscillator
*P. Palting* ..... **343**

**Properties, Dynamics, and Electronic Structure of Atoms and Molecules**

Theoretical Study of Aminoalkylation in the Mannich Reaction of Furan with Methyleneimminium Salt
*U. Maran, A. R. Katritzky, and M. Karelson* ..... **359**

Planarization of 8π Rings. I. Confirmation of a Speculation by Ermer on the Ground State of a Strained Cyclooctatetraene and Studies on Analogous Oxepins
*C. Trindle* ..... **367**

**Properties, Dynamics, and Electronic Structure of Condensed Systems and Clusters**

Indirect Adatom Interactions via III–V Semiconductor Substrates
*D. W. Schranz and S. G. Davison* ..... **377**

Theoretical Characterization of $H_2$ Adsorption on AuPt Clusters
*A. Cruz, E. Poulain, G. Del Angel, S. Castillo, and V. Bertin* ..... **399**

Volume Title Page ..... **411**

Author Index ..... **413**

Subject Index ..... **415**

Volume Table of Contents ..... **I**